

Hexanoic acid, 3,5,5-trimethyl-, isobutyl ester

Inchi:	InChI=1S/C13H26O2/c1-10(2)9-15-12(14)7-11(3)8-13(4,5)6/h10-11H,7-9H2,1-6H3
InchiKey:	FZZAUWKVCPGABZ-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CC(C)COC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	214.34

Physical Properties

Property code	Value	Unit	Source
gf	-177.38	kJ/mol	Joback Method
hf	-575.76	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	51.62	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.648		Crippen Method
mvol	201.470	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1298.00		NIST Webbook
tb	569.02	K	Joback Method
tc	752.82	K	Joback Method
tf	280.85	K	Joback Method
vc	0.764	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.23	J/mol×K	569.02	Joback Method
cpg	536.12	J/mol×K	599.65	Joback Method
cpg	553.16	J/mol×K	630.29	Joback Method
cpg	569.35	J/mol×K	660.92	Joback Method
cpg	584.73	J/mol×K	691.56	Joback Method
cpg	599.32	J/mol×K	722.19	Joback Method
cpg	613.15	J/mol×K	752.82	Joback Method
dvisc	0.0074507	Paxs	280.85	Joback Method

dvisc	0.0023501	Paxs	328.88	Joback Method
dvisc	0.0009947	Paxs	376.91	Joback Method
dvisc	0.0005113	Paxs	424.94	Joback Method
dvisc	0.0003009	Paxs	472.96	Joback Method
dvisc	0.0001952	Paxs	520.99	Joback Method
dvisc	0.0001363	Paxs	569.02	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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